Connect NMR UK: A National NMR Network for Physical and Life Sciences

Maximising the impact of UK NMR infrastructure in physical and life sciences

Coordinators

Frédéric Blanc (Liverpool)

Christina Redfield (Oxford)

Craig Butts (Bristol)

EPSRC
Engineering and Physical Sciences Research Council

Stay connected via Twitter **@ConnectNMRUK**

BBSRC bioscience for the future

MRC Medical Research Council

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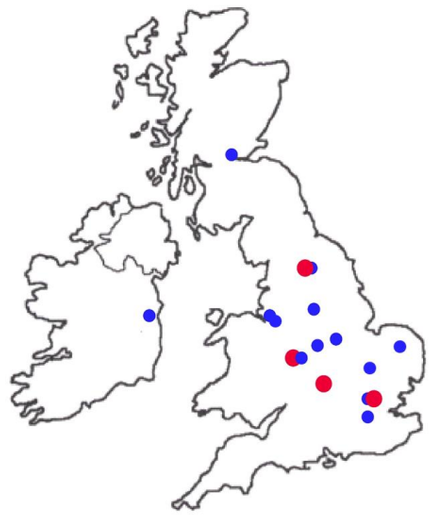

EPSRC-funded Network (£440k), 2019-2022

A network manager to facilitate knowledge of, and access to, UK NMR infrastructures and capabilities

A web portal to act as a repository and shop-window for the above

Thematic workshops and training to enable UK NMR researchers and users

Annual discussion forum to increase and share knowledge base promoting usage of the most advanced NMR technologies (in conjunction with existing UK NMR meetings)

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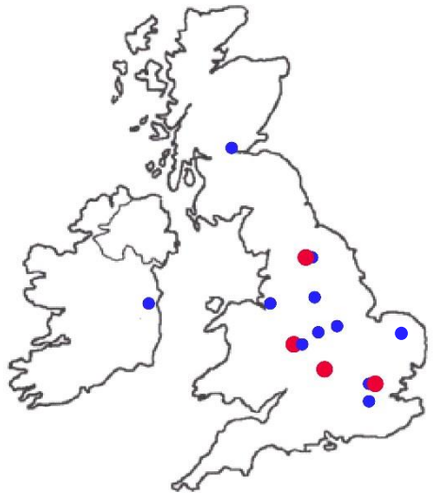

EPSRC-funded Network (£440k), 2019-2022

- Funding a full-time network manager
- Funding workshop/training/meeting activities
- 75 Travel/subsistence (£600 pp) and access costs (£1000 pp) for workshops (primarily for PhD students)
- Travel bursaries (£100 pp) for new attendees to UK NMR Meetings
- Web portal to display UK NMR capabilities, links to centres, publications etc.
- Outreach/engagement activities for Connect NMR UK at UK/EU meetings

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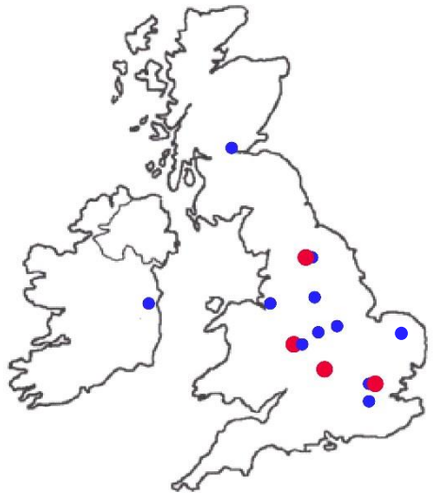

Timeline of Events

2019 Dissemination via meetings e.g. CCPN, UKMRM, NMRDG, UK Solid-state etc.
Appointment of Network Manager (June start ideally)

2020 1st Workshop and 1st Annual Discussion Forum
Topics/dates TBA – in conjunction with existing meetings/events

2021 2nd Workshop and 2nd Annual Discussion Forum

2022 3rd Workshop and 3rd Annual Discussion Forum

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Scottish High Field NMR (SHF-NMR) Centre in the School of Chemistry EPSRC 800 MHz upgrade

Participating Uni and Institutions - % of sp. time

Beatson Institute Glasgow	4%
Heriot-Watt University	4%
University of Aberdeen	4%
University of Dundee - DDU	4%
University of Edinburgh	50%
University of Glasgow	8%
University of St Andrews (incl. SS)	22%
University of Strathclyde	4%

- BMPC2 (magnet pumps and control system) upgrade – up and running (with some issues)
- Avance NEO 4 channels console with additional MAS control unit – up and running
- New Cryo-Cooling Unit/5 including nitrogen re-liquefier unit BSNL (working perfectly)
- Replacement of CP TCI helium Cryo-Probe by new generation – installed just very recently
- New generation CP TXO helium Cryo-Probe – expected installation 2019/2020
- Solids – supervised and operated by St. Andrews (prof Sharon Ashbrook and Daniel Dawson):
- MASIII Pneumatic control unit
- MASSB-TR-X/Y/1H-2.5mm DVT (Trigamma triple resonance probe) - installed
- MASSB-DR-BB/1H&19F-1.3mm DVT (high speed double resonance probe) – July/August
- MASSB-DR-BBLR/H-3.2mm DVT (top-loaded double resonance H/X probe) – July/August

Scottish NMR User Group - SNUG

Scotland

University of Glasgow

University of Aberdeen

University of Dundee

University of St Andrews

University of Strathclyde Glasgow

Heriot Watt University

The University of Edinburgh

SNUG – an association of Scottish NMR laboratories set up in 2015 to facilitate:

- access to NMR instrumentation for academic and industrial users
- sharing of resources - hardware & expertise
- application for funds to maintain our first-class instrumentation
- educational activities for academia and industry
- outreach and high school activities.

http://www.snug.ac.uk/,

- will list of our resources and will consists of public and private pages.
- SNUG meeting at Loch Tay, 2015 - 2018
- 5th SNUG meeting this year at Loch Ard, August 28th – 30th, 2019

Nottingham High Field Facility

The University of Nottingham
UNITED KINGDOM · CHINA · MALAYSIA

Ascend 800MHz

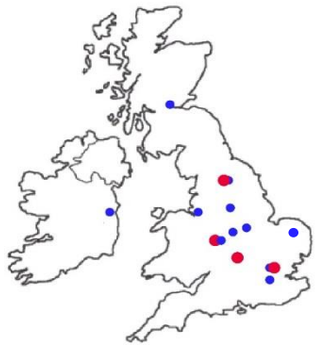
5 Channel NEO Console – Installed December 2019

<u>Solution</u>
- 5 mm QCI Helium cryoprobe
- 1.7 mm HCN Helium cryoprobe – Delivery August 2019

<u>Solid state</u>
- 1.3 mm HCN – Install Monday
- 3.2 mm HCN – Delivery August 2019
- 3.2 mm HX – Delivery August 2019
- 3.2 mm HX low gamma – Delivery August 2019

All enquiries welcome
Contact: huw.williams@nottingham.ac.uk
Web: www.nottingham.ac.uk/analytical/

High-Field Biomolecular NMR Facility
University of Sheffield



Funding received from EPSRC: £0.9M

Equipment upgrade to existing 800MHz:
BMPCII
Neo 4-channel console
5mm TCI cryoprobe; BSNL
Temperature-controlled SampleJet (480 samples)

Projects:
Just starting some high-throughput biotechnology

The University Of Sheffield.

RESONS Biological NMR

Liverpool 800 MHz NMR upgrade

Research interests include:

Materials chemistry (supramolecular assemblies, energy materials, heterogeneous catalysis, oxides);

Life science – physical science interfaces (homogeneous catalysis, medicinal chemistry, green energy, chemical shift imaging);

Industrial biotechnology and synthetic biology (industrial biomaterials, enzymes for biotechnology);

Health, personalised medicine and drug (medicinal chemistry, neurodegenerative amyloid diseases, metabolic diseases, cancer, ageing and chronic diseases);

NMR research expertise include solids, quadrupolar nuclei;

Funding secured by Dr. F. Blanc (PI) and Drs. I. Barsukov / J. Iggo / K. Luzyanin / Prof. L.-Y. Lian (CoIs); Across the Faculty of Science and Engineering and the Faculty of Health and Life Sciences.

Liverpool 800 MHz NMR upgrade: equipment

Upgrade of the biomolecular solution state 800 MHz system in the NMR Centre for Structural Biology to a **multi-purpose biomolecular and chemistry** spectrometer;

New triple resonance + NEO console and BMPC;

Extended solution, and **new** solid and soft matter NMR capabilities;

Solution: 5 mm ^{13}C,^{15}N-optimised cryoprobe (“TCO”, unique at this field ?); 5 mm double resonance probe with broad band capabilities (^{31}P – ^{109}Ag) and extended vt range (-150 to 150 °C) (“BBO”); refrigerated autosampler with 6 x 96 5 mm tubes (”Sample Jet”) in addition to the existing 5 mm ^{1}H-optimised cryoprobe (“TCI”).

Solids: 1.3 mm double resonance probe with broad band (^{31}P – ^{15}N) and ^{19}F capabilities; 1.9 mm triple resonance tri-gamma probe (^{13}C < X < ^{31}P; ^{15}N < Y < ^{23}Na); a unique 3.2 mm single resonance probe (^{31}P – ^{13}C) with a balance circuit (for enhanced rf); 3.2 mm double resonance probe with low-g capabilities (^{13}C/^{23}Na – ^{109}Ag); vt range on all probes -50 to 80 °C.

Soft matter: 4 mm HR-MAS ^{13}C-optimised probe, vt range -20 to 80 °C.

Operation expected to start in Dec 2019.

Liverpool 800 MHz NMR upgrade: access & costings

Facility Management Committee co-chaired by Dr. F. Blanc and Prof. L.-Y. Lian with 2 UoL members and 2 external members (e.g. directors of other very/ultra high field facilities);

Simple 1 page peer review process for access;

Up to 30% of usage external to UoL;

Minimum allocation of time is 1 day;

3-month cycle of solution and solid (split 50:50 between both modes, split 50:50 between physical- and life-sciences);

NMR-trained users will run their own experiments, supported by existing experimental officers;

Access charges to recover costs will apply: £250 per day (charges should be included in grant costings as “directly incurred”for the time being);

Contact: Dr. F. Blanc (frederic.blanc@liverpool.ac.uk) and Prof. L.-Y. Lian (Lu-Yun.Lian@liverpool.ac.uk)

UNIVERSITY OF BIRMINGHAM

UKMRM meeting, University of York, 20 June 2019

HWB·NMR

Henry Wellcome Building for Biomolecular NMR Spectroscopy

GHz for the UK

Contact: Sara Whittaker

www.nmr.bham.ac.uk

UNIVERSITY OF BIRMINGHAM

HWB·NMR

UKRI-funded equipment

5 mm TCI cryogenic probe at 1.0 GHz
(with temperature-controlled SampleJet)

- for ^{1}H-optimised & ^{13}C/^{15}N-sensitive direct detection
- shaped tube compatible (optimum sensitivity for salty samples, 350 µl volume)
- biomolecules in solution state

- 1.0
- GHz

Low-volume cryogenic probe at 1.0 GHz? - tbd

- for ^{1}H-optimised & ^{13}C/^{15}N-sensitive direct detection
- for mass-limited samples (proteins, tracer-based metabolism/metabolomics, natural products etc)

1.3 mm CP-MAS H/C/N probe at 900 MHz

- up to 67 kHz rotation frequency (standard bore magnet)
- for biomolecular solid-state NMR

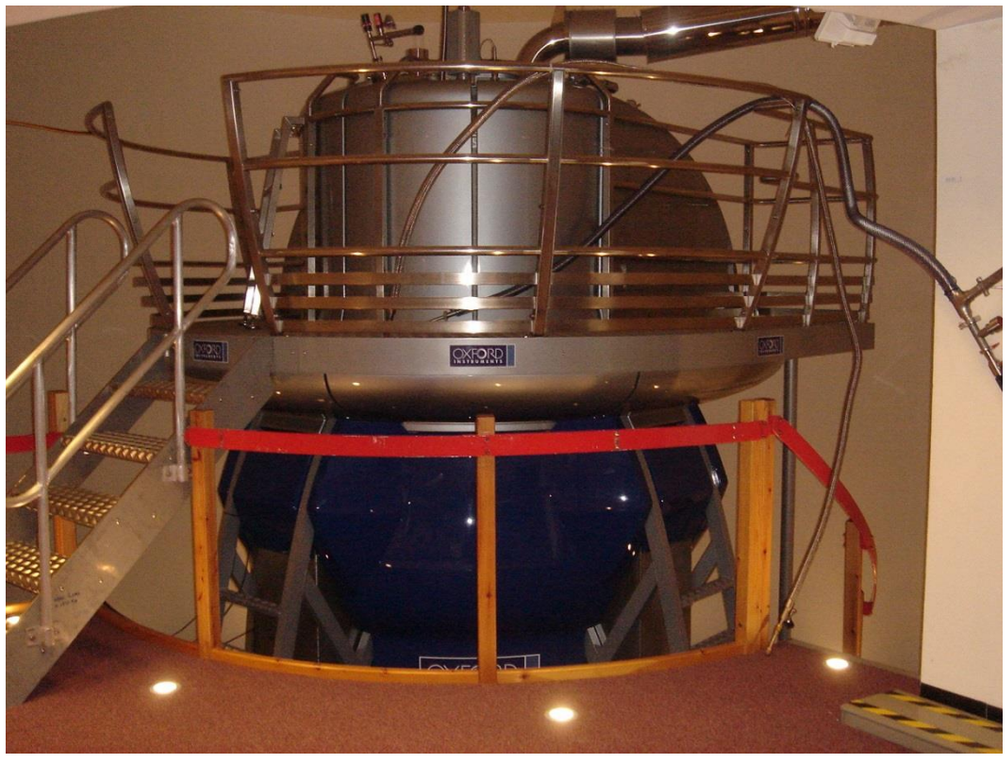
- 900 MHz

- 800 MHz

Open access Wellcome Trust-funded use until 2023
(50% of available time *free* across GHz, 900 MHz & 800 MHz)

Contact: Sara Whittaker

www.nmr.bham.ac.uk



950 MHz Spectrometer

- 22.3 Tesla Oxford Instruments Company magnet installed in 2005.
- Magnet has excellent characteristics including minimal field drift (-3.9Hz/hr)
- Upgraded with a Bruker Avance III console and RT 5mm TXI probe in 2016 (funded internally).

EPSRC-funded upgrade to Oxford 950

- ~£500K upgrade
  - 5mm TCI CryoProbe (suitable for 3mm and ‘shaped’ tubes)
  - Cooled SampleJet sample changer
- Tests carried out at the Crick suggest a ~2-3 fold improvement in S/N for typical protein samples.
- The SampleJet will increase throughput allowing compound screening and ligand titrations.
- Timeframe – SampleJet (installed Feb 2019), CryoProbe (June/July 2019)

Access to the 950 MHz at Oxford

- Although this upgrade only represents ~20% of spectrometer value, we have committed to providing 50% of time to external users.

- We put forward a 'hub and spokes' model with prospective users from Cambridge, Kent, London, Portsmouth, Southampton, Bath, Bristol, Exeter & Cardiff but we will accept requests for time from all UK NMR groups.

- We envisage a mixed model with some free and some paid access (~£100-£150 per day).

- No firm decisions about an access model have been made.
  - We are open to operating within a UK NMR 'network'.
  - We believe there is a demand from some groups for large blocks of NMR time at relatively short notice (when samples are available).

- Contact person – christina.redfield@bioch.ox.ac.uk

Oxford 950 for Physical Sciences

- University of Oxford internal funding provides for 40 days of free instrument time (over 2 years). Pilot study to assess demand

- For those "*who have research questions in the physical sciences that would benefit from ultra-high-field NMR*"

- Management committee: Profs Christina Redfield, Tim Claridge & Craig Butts

- Applications undergo "light-touch" review prior to time allocation

Contact: christina.redfield@bioch.ox.ac.uk

Oxford 950 for Physical Sciences